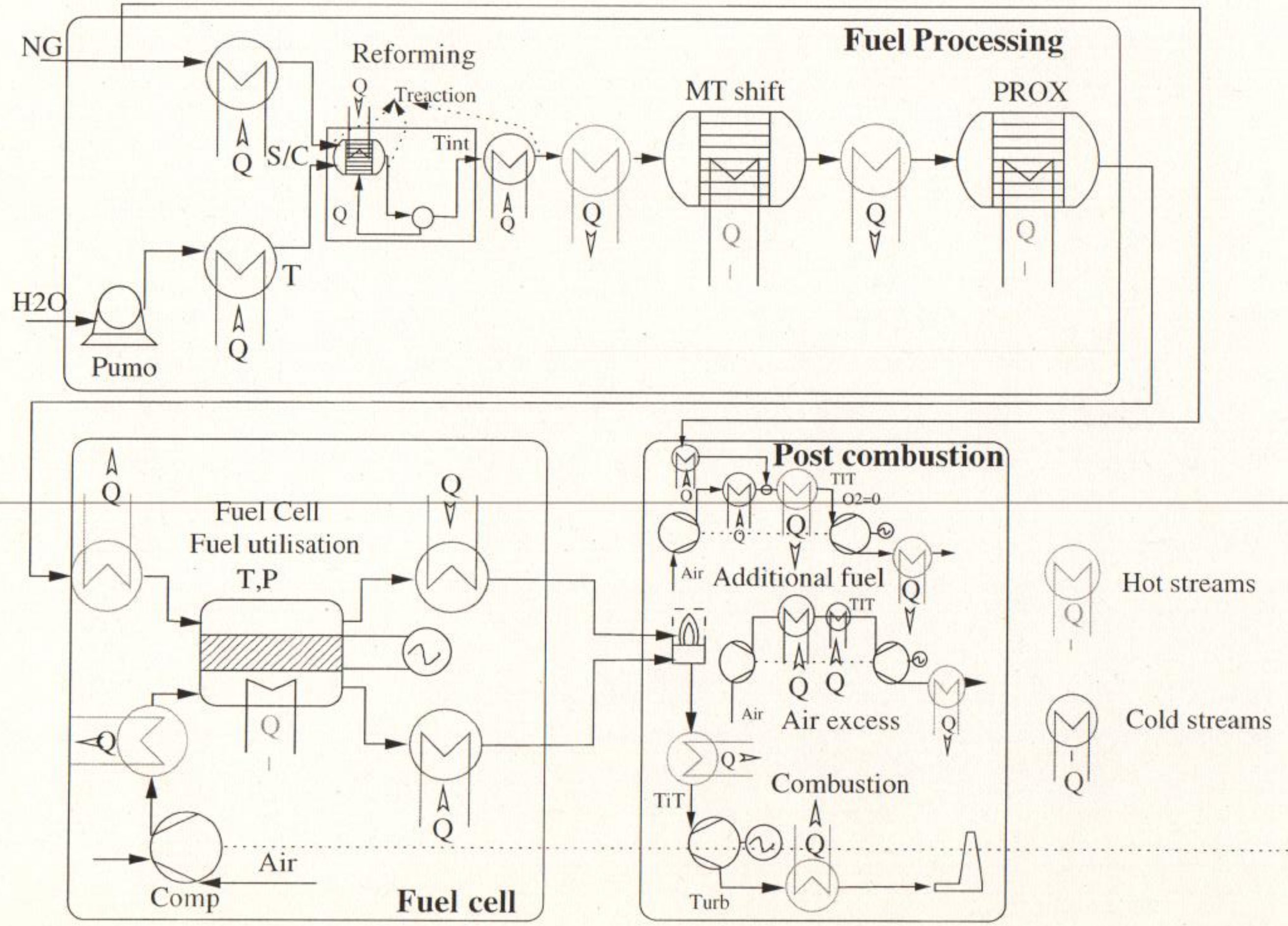
PEMFC system Energy Flow Diagram



Optimization of a fuel cell system using process integration techniques

François Marechal, Julien Godat
Laboratory of Industrial Energy Systems
LENI STI-ISE-EPFL
Swiss Federal Institute of Technology - CH-Lausanne
mailto:francois.marechal@epfl.ch

OUTLINE

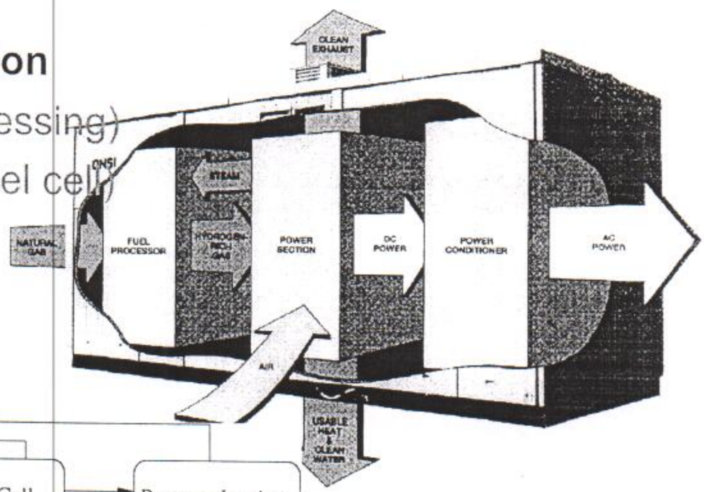
- **Problem Statement**
- **Tools and methodology**
  - Modelling
  - Optimisation
- **Application**
- **Results and outcome**
- **Conclusions**
  - Methods
  - System
- **Future work**

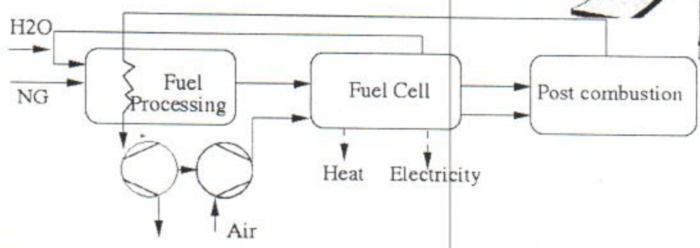
EPFL

Problem statement

PEM Fuel cell system

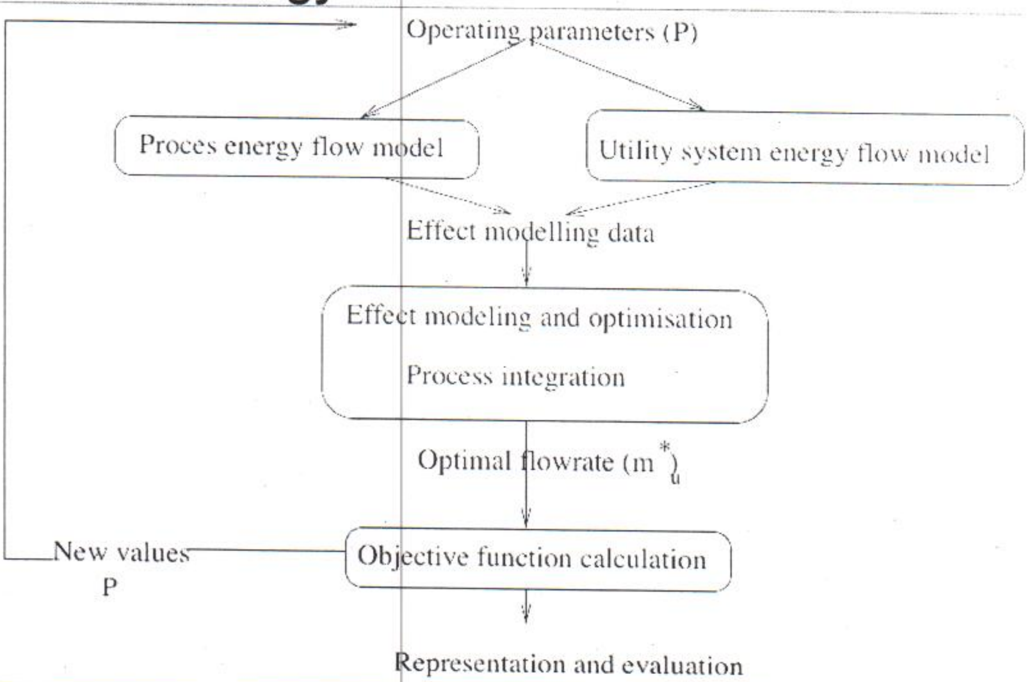
- **High level of integration**
  - Chemical (fuel processing)
  - Electro-chemical (fuel cell)
  - Thermal



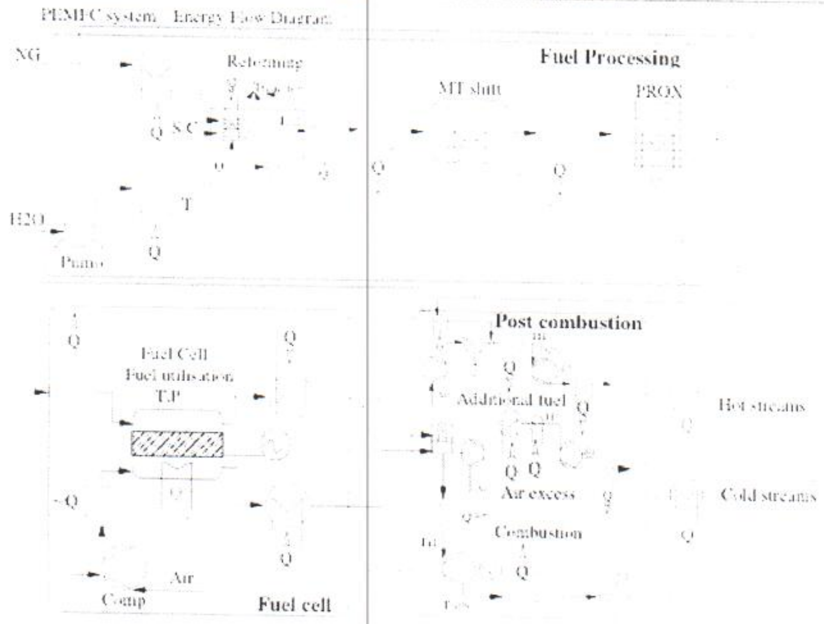


EPFL

Methodology



Process energy flow model



Energy Flow model : Modelling Tool

- **Tool : BELSIM -VALI (http://www.belsim.com)**
  - Thermo-physical properties & models
  - Heat and Mass Balances
  - Liquid-Vapor equilibrium
    - State specification
  - Equipment modelling
    - Heat exchangers
    - Atomic balances
    - Reactors
      - Equilibrium + ΔT_{eq}
  - Model customising tools
    - programming
  - Equation solver
    - Optimisation
    - Over -specified calculations (least square approach)
    - Bounds

Modelling assumptions

- **Reformer + shift**
  - T and P to be optimised
  - Steam to carbon ration to be optimised
    - The endothermic steam methane reforming $CH_4 + H_2O \rightleftharpoons 3H_2 + CO (\Delta H_r = 206.11 kJ/mol)$
    - The exothermic water gas shift $CO + H_2O \rightleftharpoons CO_2 + H_2 (\Delta H_r = -41.2 kJ/mol)$
- **Preferential oxidation**
  - Catalytic combustion (1 mol O2/ 1 mol CO)

$$CO + O_2 \rightleftharpoons CO_2$$

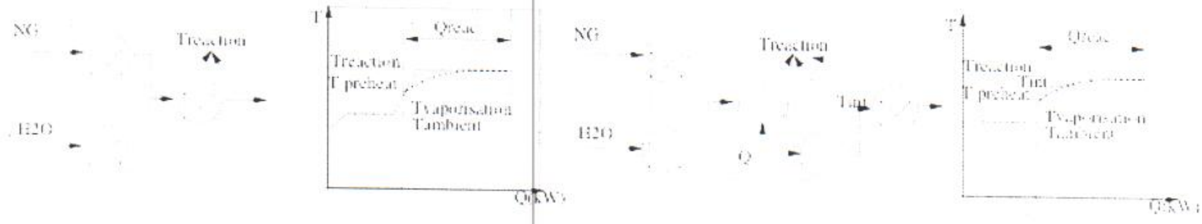
$$H_2 + \tfrac{1}{2}O_2 \rightleftharpoons H_2O.$$

Fuel Cell model

- Nernst potential (V) :
  $U_{Nernst} = U^0_{Nernst}(T_{cell}) + \frac{RT_{cell}}{2F} Ln(\frac{Y^{H_2}_{anode} Y^{O_2}_{anode}}{Y^{H_2O}_{anode}}) + \frac{RT_{cell}}{1F} Ln(P_{cell})$
- Cell voltage (V): $V_{cell} = U_{Nernst} - R_{cell} i_{cell}$
- Hydrogen flow rate through the membrane: $n^{H_2}_{i,cathode} = \frac{I_{cell}}{2*F}$
- Cell current (A): $I_{cell} = i_{cell} \cdot A_{cell}$
- Cell power (W): $P_{cell} = V_{cell} I_{cell}$
- Fuel cell power(W): $P_{FC} = P_{cell} \cdot N$
- Hydrogen oxidation at the cathode : $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$
- Energy Balance :
  $\sum_{i=1}^{inlets} f_i * h_i(T_{cell}, P_{cell}) - \sum_{o=1}^{outlets} f_o * h_o(T_{cell}, P_{cell}) = E_{FC} + Q^-_{FC}$
- Fuel utilisation : $\eta_{comb} = \frac{n^{H_2}_{i,anode} - n^{H_2}_{o,anode}}{n^{H_2}_{i,anode}}$

Process Integration

- **List of Hot and Cold stream**
  - Appropriate definition of energy requirement



- **Utility system => unknown**
  - Additional firing
  - Preheating
  - Gas turbine

Process integration

- DTmin in exchangers
- No prespecified interconnections
- Additional firing
- Gas turbine integration
- Optimisation
- Graphical representation

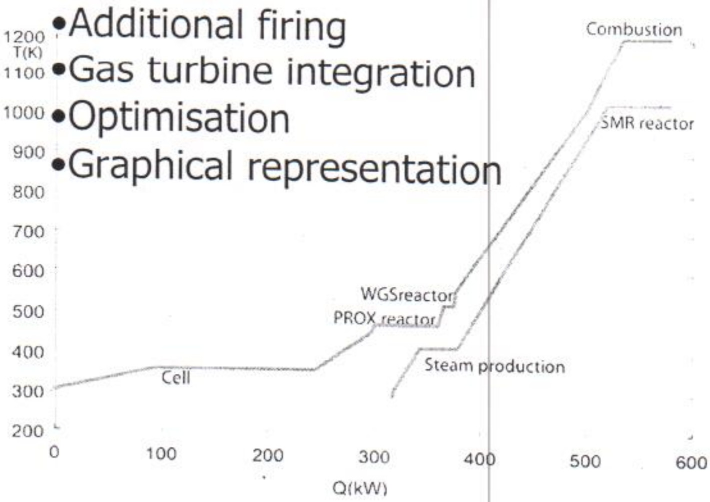


Table 1
The fuel processing subsystem streams. Syngas composition $CO, H_2O, H_2, CO_2, CH_4$

#		Description	T_{in}	T_{target}	Flow type
1	Cold	Water preheating for SMR reaction (including liquid water preheating, the vaporisation and the steam superheating)	20 °C	[illegible]	H_2O
	Cold	Methane preheating for SMR reaction	25 °C	[illegible]	CH_4
	Hot	The stream between the SMR and WGS reactions	[illegible]	[illegible]	syngas
	Hot	The stream between the WGS and PROX reactions	[illegible]	[illegible]	syngas
	Hot	The generated heat by the WGS reaction	[illegible]	[illegible]	Heat
	Hot	The generated heat by the PROX reaction	[illegible]	[illegible]	Heat
	Cold	The required heat by the SMR reaction	[illegible]	[illegible]	Heat

Table 2
The PEMFC subsystem streams. Flue gas composition : H_2O, CO_2, O_2, N_2

#		Description	T_{in}	T_{target}	Flow type
8	Hot	The stream between the fuel processing subsystem outlet and PEMFC inlet	[illegible]	[illegible]	syngas
9	Hot	The air compressor outlet cool down to the cathode inlet	[illegible]	[illegible]	Air
10	Hot	The stream between the cathode outlet and the water separator	[illegible]	25 °C	flue gas
11	Hot	The generated heat by the PEMFC	[illegible]	[illegible]	Heat

Table 3
The post combustion subsystem streams

#		Description	T_{in}	T_{target}	Flow type
12	Cold	The air preheating for the combustion	25 °C	[illegible]	flue gas
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15	Hot	The gases combustion stream after the exchanger	[illegible]	[illegible]	flue gas

MILP formulation

$$\min_{R_r, y_w, f_w, Wel, Wel_s} \left(\sum_{w=1}^{n_w} (C2_w f_w) + Cel\,Wel - Cel_v Wel_s \right) \cdot t_{op}$$

Fixed maintenance

$$+ \sum_{w=1}^{n_w} (C1_w y_w) + \frac{1}{\tau} \sum_{w=1}^{n_w} (ICF_w y_w + ICP_w f_w) \quad (1)$$

Investment

Subject to Heat balance of the temperature intervals

$$\sum_{w=1}^{n_w} f_w q_{w,r} + \sum_{i=1}^{n} Q_{i,r} + R_{r+1} - R_r = 0 \qquad \forall r = 1, \ldots, n_r \quad (2)$$

Electricity consumption

$$\sum_{w=1}^{n_w} f_w w_w + Wel - Wc \geq 0$$

Electricity production

$$\sum_{w=1}^{n_w} f_w w_w + Wel - Wel_s - Wc = 0$$

Technology selection

$$fmin_w y_w \leq f_w \leq fmax_w y_w \qquad \forall w = 1, \ldots, n_w y_w \in 0, 1$$

Feasibility

$$Wel \geq 0, Wel_s \geq 0 \quad (6)$$

$$R_1 = 0, R_{n_{r+1}} = 0, R_r \geq 0 \qquad \forall r = 1, \ldots, n_{r+1} \quad (7)$$

Optimisation problem

$$\underset{P}{Min}\ \eta_e(P, \dot{m}_u^*) = \frac{\dot{E}_{FC}(P) + \dot{E}_{GT}(P, \dot{m}_u^*)}{\dot{m}_{FC} \cdot LHV_{NG} + \dot{m}_{NG_{add}}(P, \dot{m}_u^*) \cdot LHV_{NG} + \dot{m}_{O_2}(P) \cdot \dot{E}_{O_2}} \quad (1)$$

with

$$\dot{m}_u^*(P) = \underset{\dot{m}_u, y_u}{Min}\ \eta_e(P, \dot{m}_u) \quad (2)$$

subject to (3)

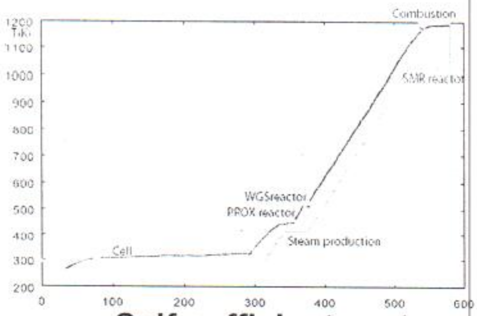
Heat cascade constraint (4)

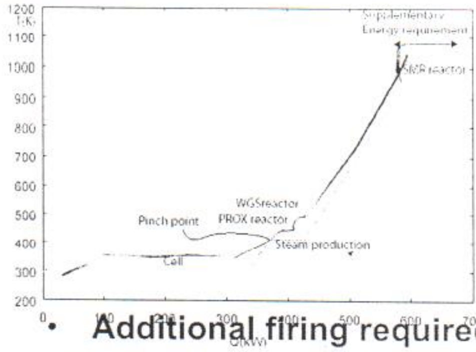
Mechanical power balance (5)

where

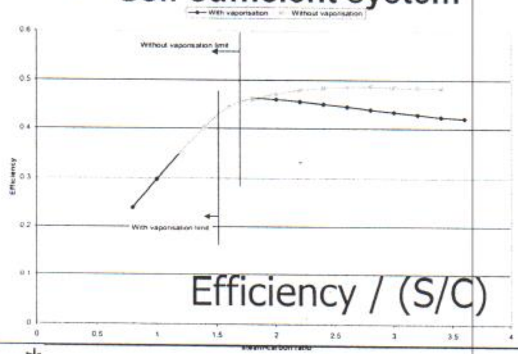
$\dot{E}_{FC}$	is the electricity production by the fuel cell
$\dot{E}_{GT}$	is the net electricity production by the integrated gas turbine system
$\dot{m}_{FC}$	is the flowrate of natural gas entering the fuel processing units
$\dot{m}_{NG_{add}}$	is the flowrate of additional natural gas used to increase the power of the gas turbine sub-system
LHV_{NG}	is the lower heating value of the natural gas.
$\dot{m}_{O_2}$	is the pure oxygen flow used in the PROX reactor
$\dot{E}_{O_2}$	is the energy consumption of the pure oxygen used in the system (here we considered an amount of energy of 300 kWh/ton of O_2.
$\dot{m}_u$	represent the flowrates in the utility system
y_u	represent the integer variable representing the use or not of the utility stream u
P	represent the decision variables of the main problem

Self sufficient system

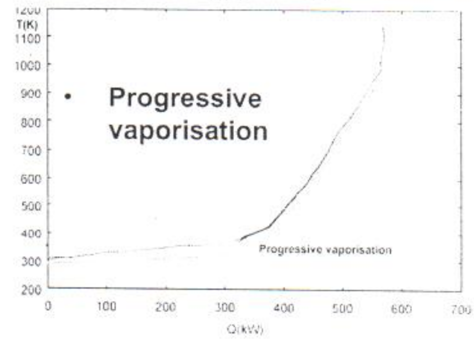




- Self sufficient system
- Additional firing required



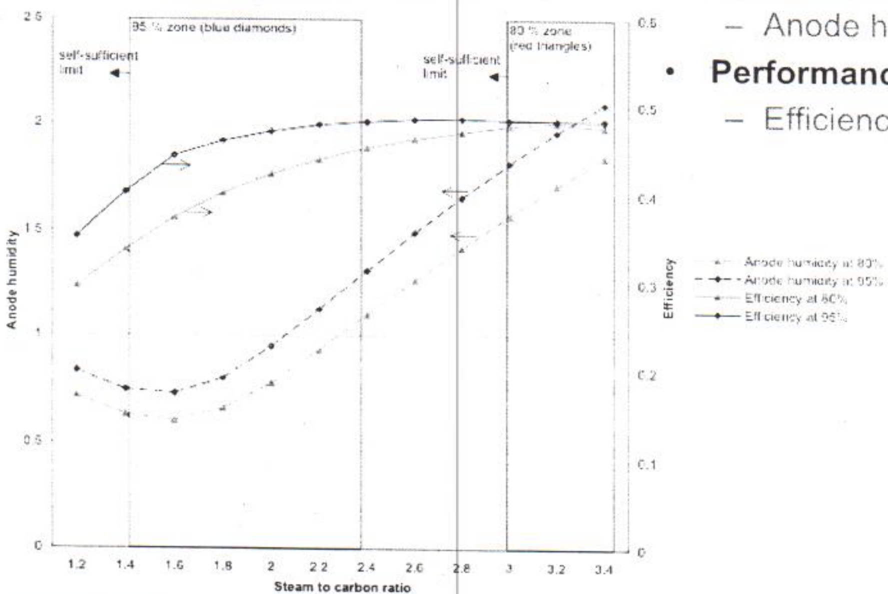
Efficiency / (S/C)



- Progressive vaporisation

Sensitivity analysis analysis

- Fuel utilisation sensitivity



- Operating conditions
  - Anode humidity
- Performances
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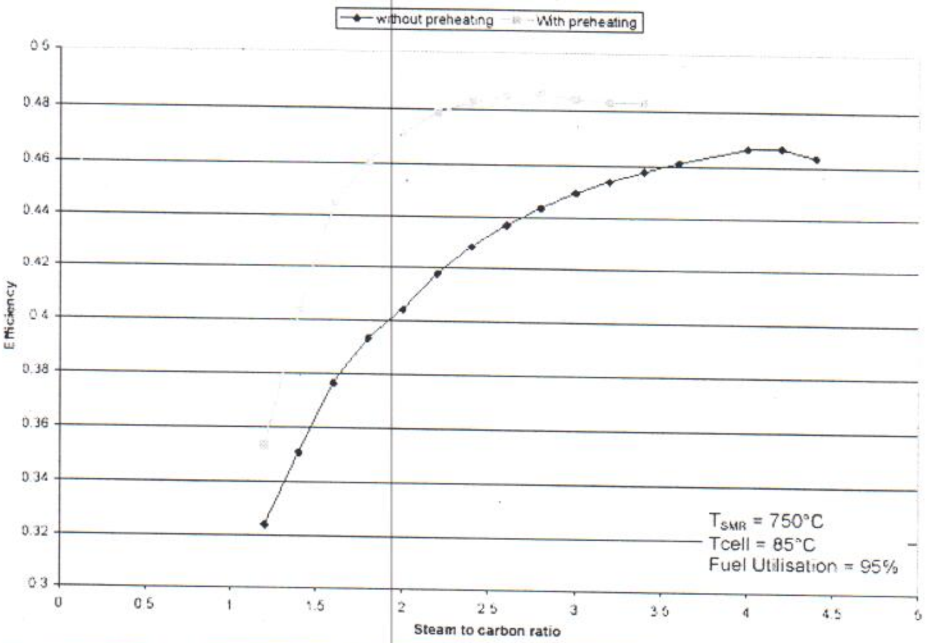
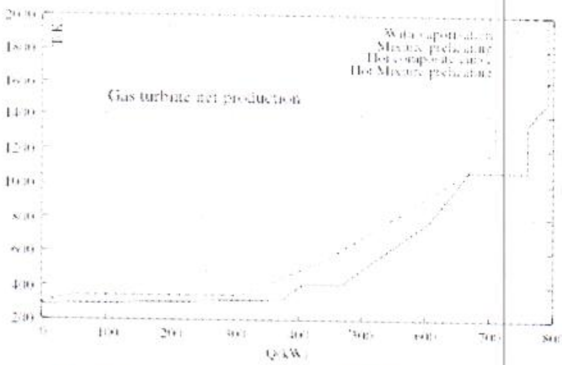
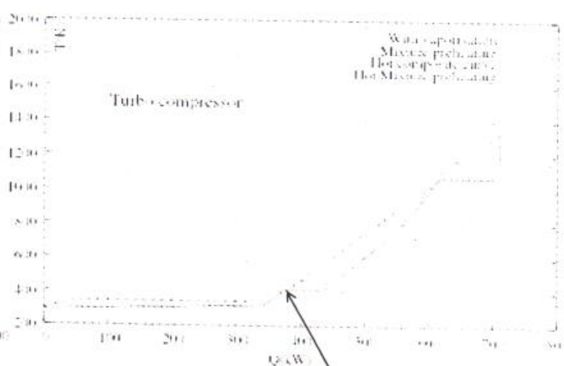
Effect of the combustion preheating



Process modifications

- With gas turbine
- With turbo expander





Separate steam production
Or fuel saturation

Pinch activated

Separate steam production
Produces a penalty (1.1 % eff_{el})

Tref = 800°C, S/C = 2.6

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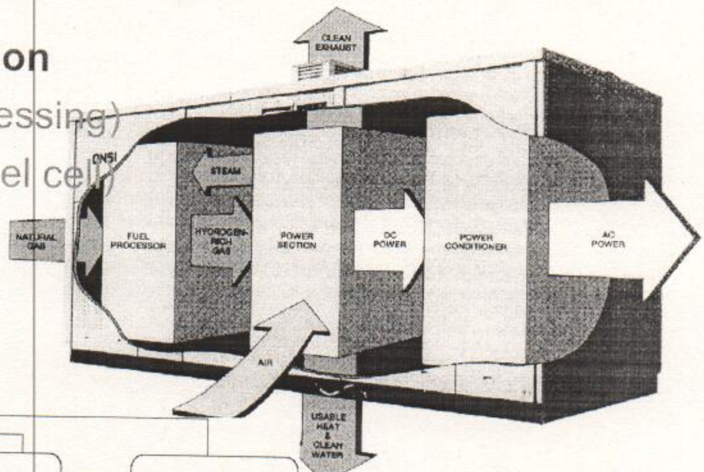

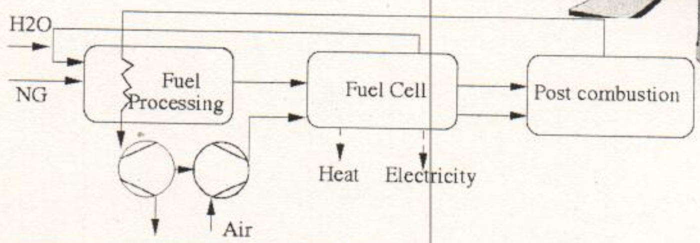

EPFL

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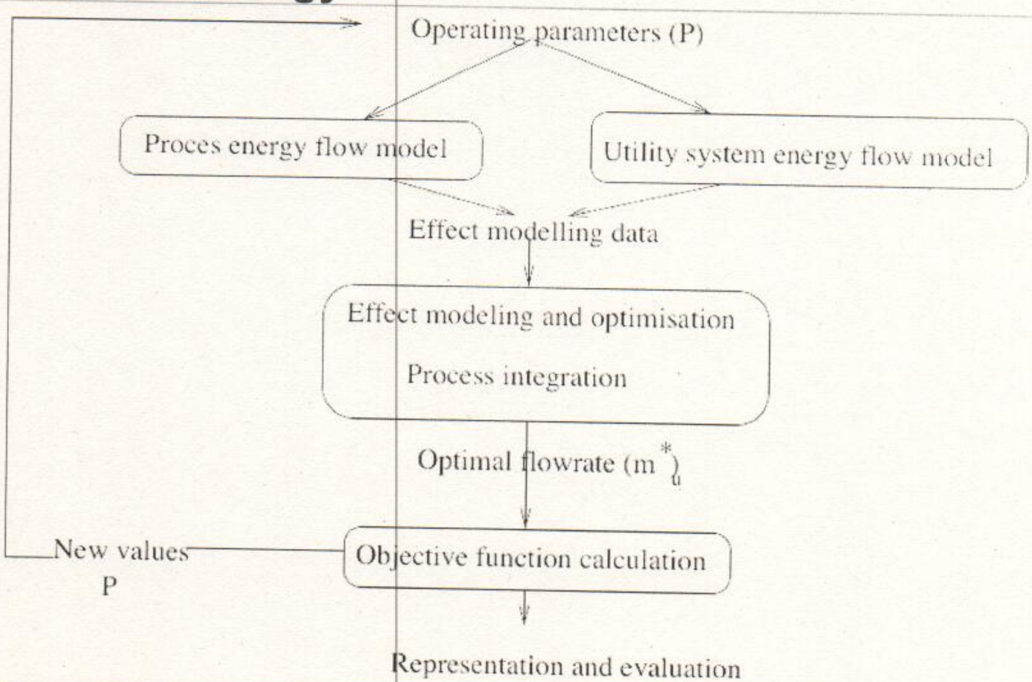

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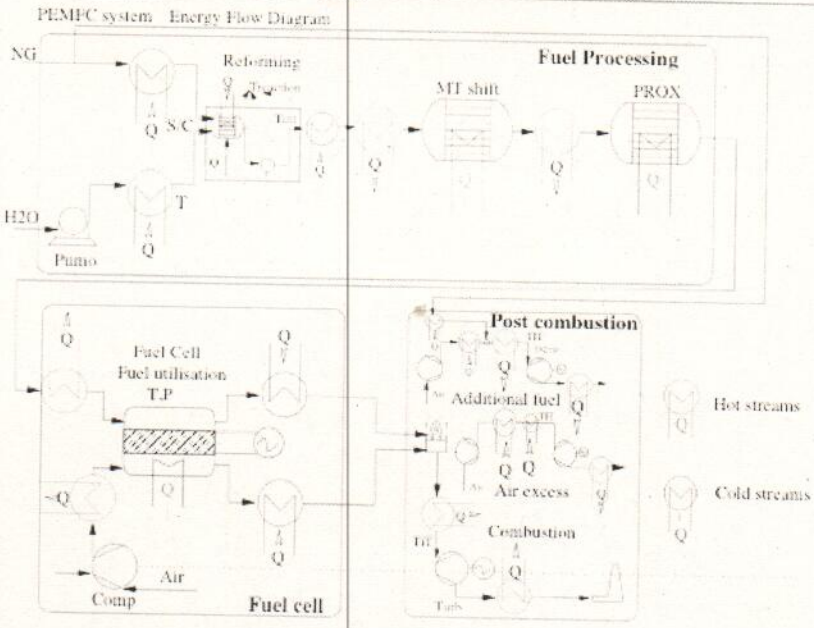

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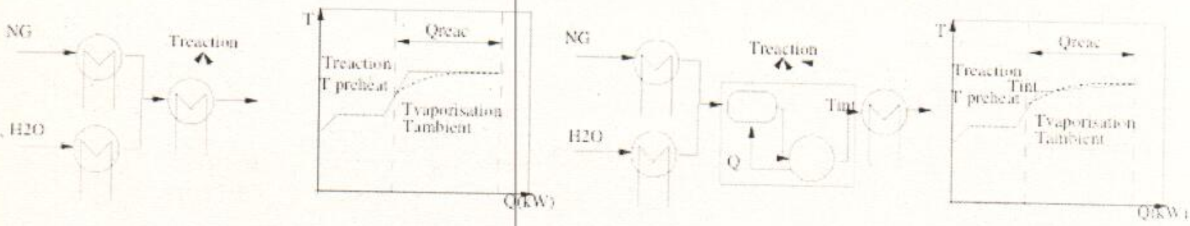
- Fuel utilisation : $\eta_{comb} = \frac{n^{H_2}_{i,anode} - n^{H_2}_{o,anode}}{n^{H_2}_{i,anode}}$

Process Integration

- **List of Hot and Cold stream**
  - Appropriate definition of energy requirement



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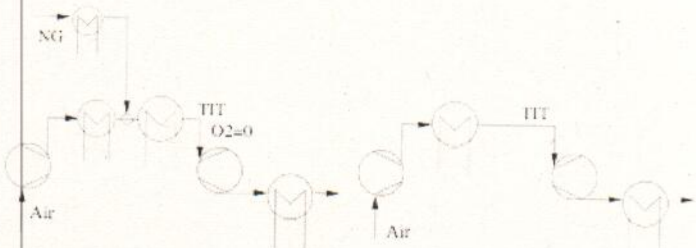

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Process integration

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- Additional firing
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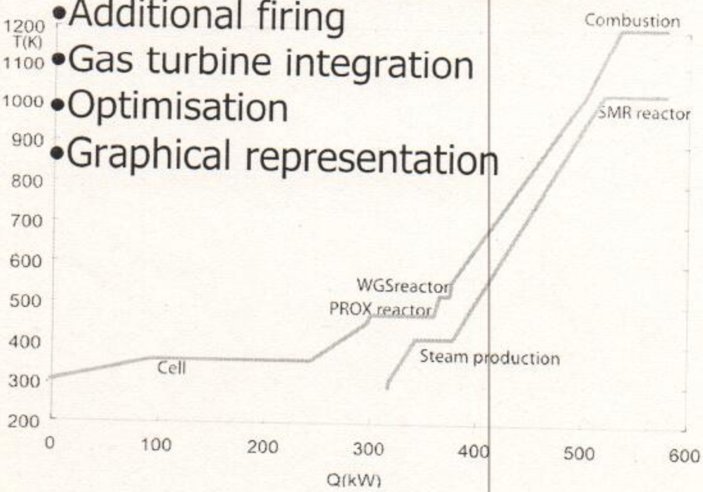

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The Fuel processing subsystem streams. Syngas composition $CO, H_2O, H_2, CO_2, CH_4$

#		Description	T_{in}	T_{target}	Flow type
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	Hot	The stream between the WGS and PROX reactions	[illegible]	[illegible]	syngas
	Hot	The generated heat by the WGS reaction	[illegible]	[illegible]	Heat
	Hot	The generated heat by the PROX reaction	[illegible]	[illegible]	Heat
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Table 2
The PEMFC subsystem streams, Flue gas composition : H_2O, CO_2, O_2, N_2

#		Description	T_{in}	T_{target}	Flow type
8	Hot	The stream between the fuel processing subsystem outlet and PEMFC inlet	[illegible]	[illegible]	syngas
9	Hot	The air compressor outlet cool down to the cathode inlet	[illegible]	[illegible]	Air
10	Hot	The stream between the cathode outlet and the water separator	[illegible]	35°C	flue gas
11	Hot	The generated heat by the PEMFC	[illegible]	[illegible]	Heat

Table 3
The post combustion subsystem streams

#		Description	T_{in}	T_{target}	Flow type
12	Cold	The air preheating for the combustion	35°C	500°C	flue gas
13	Cold	The depleted fuel preheating for the combustion	[illegible]	500°C	syngas
14	Hot	The generated heat by the combustion	[illegible]	[illegible]	flue gas
15	Hot	The gases combustion stream after the expander	[illegible]	120°C	flue gas

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MILP formulation

Operating cost

$$\min_{R_r, y_w, f_w, Wel, Wel_s} \left(\sum_{w=1}^{n_w} (C2_w f_w) + CelWel - Cel_v Wel_s \right) * t_{op}$$

Fixed maintenance

$$+ \sum_{w=1}^{n_w} (C1_w y_w) + \frac{1}{\tau} \sum_{w=1}^{n_w} (ICF_w y_w + ICP_w f_w) \quad (1)$$

Investment

Subject to Heat balance of the temperature intervals

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Electricity consumption

$$\sum_{w=1}^{n_w} f_w w_w + Wel - Wc \geq 0$$

Electricity production

$$\sum_{w=1}^{n_w} f_w w_w + Wel - Wel_s - Wc = 0$$

Technology selection

$$fmin_w y_w \leq f_w \leq fmax_w y_w \qquad \forall w = 1, ..., n_w y_w \in 0, 1$$

Feasibility

$$Wel \geq 0, Wel_s \geq 0 \quad (6)$$

$$R_1 = 0, R_{n_{r+1}} = 0, R_r \geq 0 \qquad \forall r = 1, ..., n_{r+1} \quad (7)$$

Optimisation problem

$$\underset{P}{Min}\ \eta_e(P, \dot{m}_u^*) = \frac{\dot{E}_{FC}(P) + \dot{E}_{GT}(P, \dot{m}_u^*)}{\dot{m}_{FC} \cdot LHV_{NG} + \dot{m}_{NG_{add}}(P, \dot{m}_u^*) \cdot LHV_{NG} + \dot{m}_{O_2}(P) \cdot \dot{E}_{O_2}} \quad (1)$$

with

$$\dot{m}_u^*(P) = \underset{\dot{m}_u, y_u}{Min}\ \eta_e(P, \dot{m}_u) \quad (2)$$

subject to

(3)

Heat cascade constraint (4)

Mechanical power balance (5)

where
- $\dot{E}_{FC}$ is the electricity production by the fuel cell
- $\dot{E}_{GT}$ is the net electricity production by the integrated gas turbine system
- $\dot{m}_{FC}$ is the flowrate of natural gas entering the fuel processing units
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- LHV_{NG} is the lower heating value of the natural gas.
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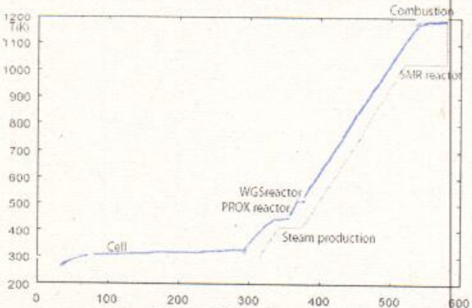
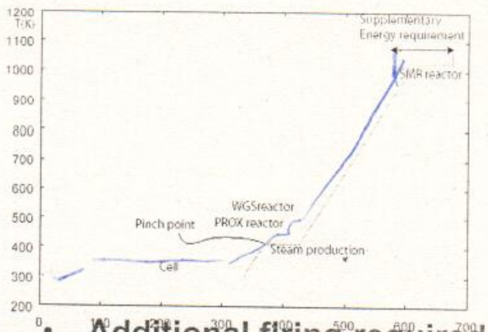
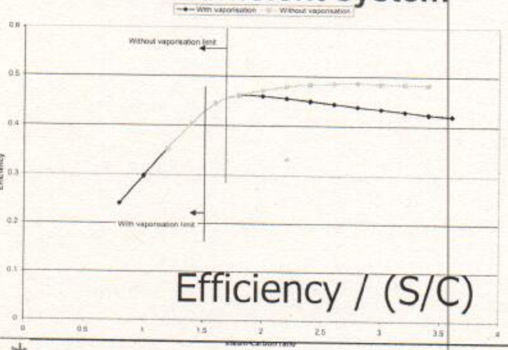
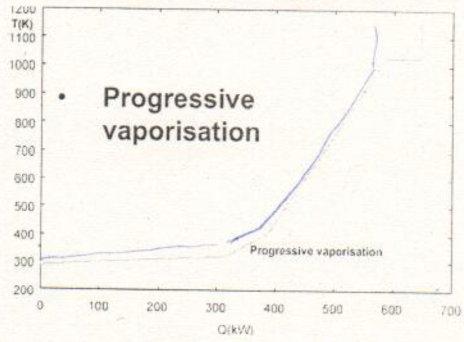
Self sufficient system





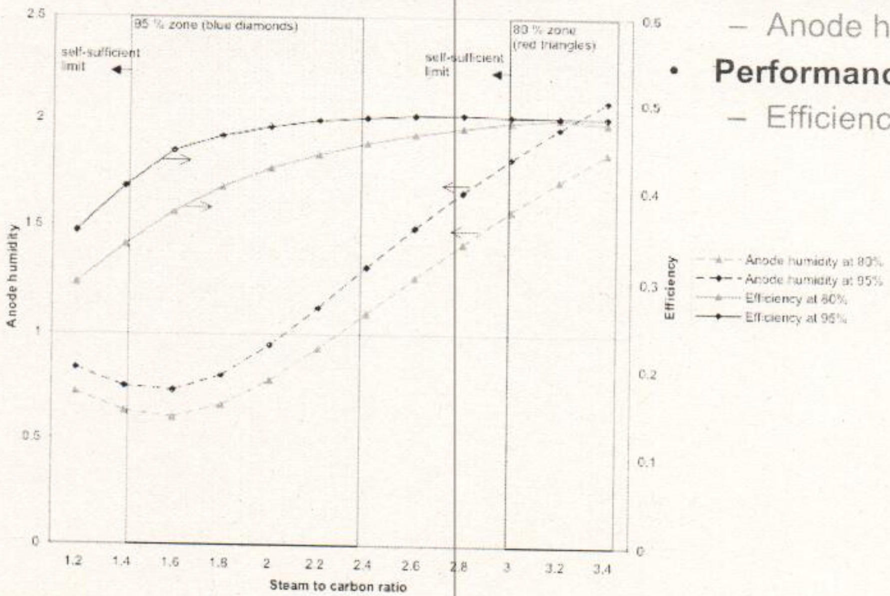
- Self sufficient system
- Additional firing required





Sensitivity analysis analysis

- Fuel utilisation sensitivity



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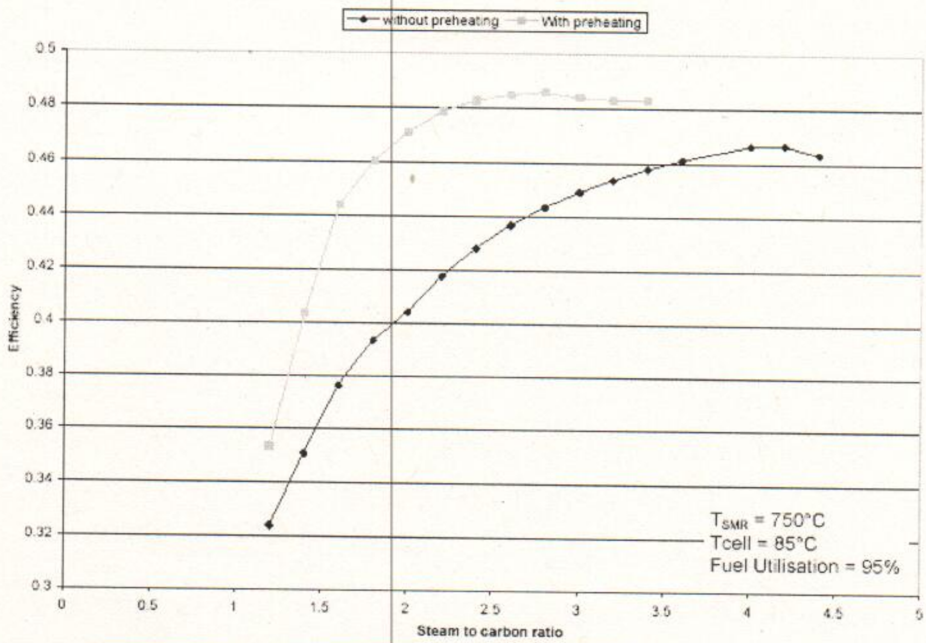
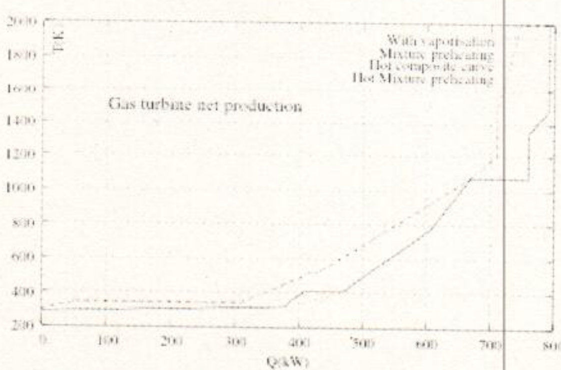
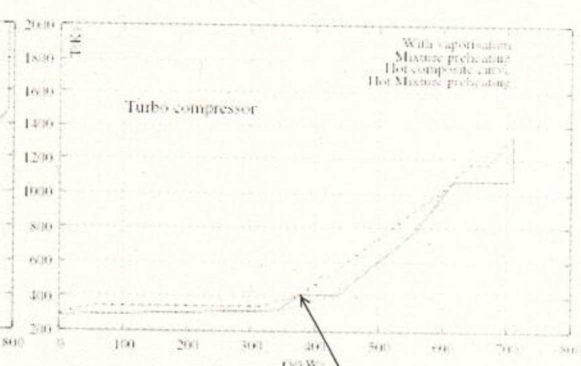
Effect of the combustion preheating



Process modifications

- With gas turbine
- With turbo expander





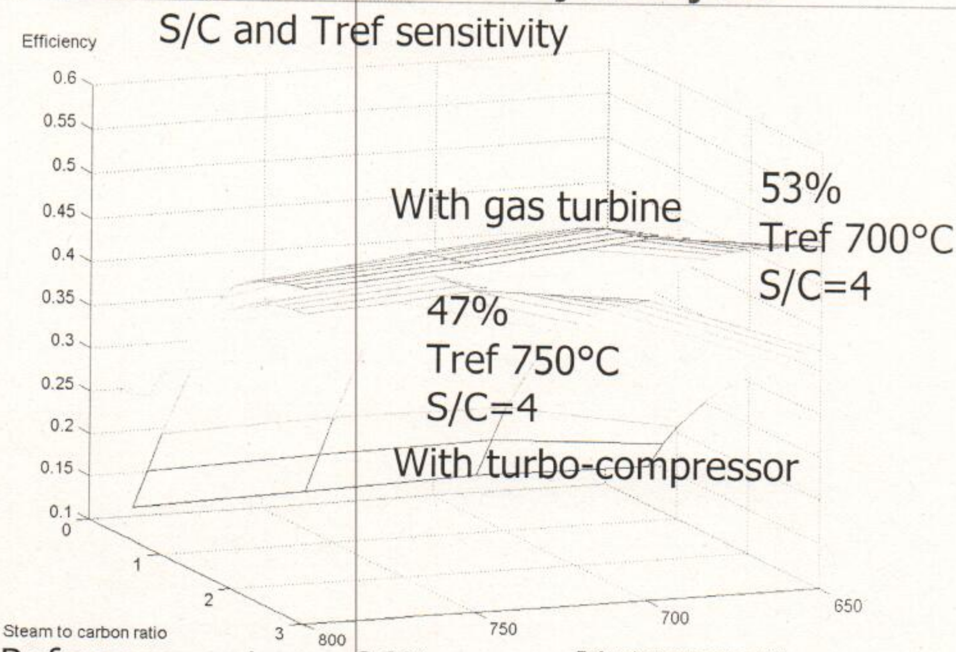
Separate steam production
Or fuel saturation

Pinch activated

Separate steam production
Produces a penalty (1.1 % eff_{el})

Tref = 800°C, S/C = 2.6

Optimisation - sensitivity analysis



Reference system : 36%

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Conclusions

- **Combined use of process models and process integration**
  - Process modifications
  - Process design specification
  - Process thermo-economic optimisation
- **Modelling tool**
  - Energy flow modelling (no heat exchange specified)
  - Equation solver
    - Bounds, optimisation
    - ? Initialisation
- **Process integration**
  - Heat exchanger network model
  - Optimisation formulation (MILP) => flows
  - Graphical representation => creativity

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Tools

- **BELSIM VALI**
  - www.belsim.com
    - Data réconciliation and process models
    - Equation solver
    - Modular approach
- **EASY (Energy Analysis and SYnthesis)**
  - mailto:francois.marechal@epfl.ch (LENI)
    - Process integration & optimisation
- **MATLAB**
    - algorithm implementation
    - Data transfer and management
- **QMOO**
  - For future multi-objective optimisation
    - Leniwww.epfl.ch

Future work

- **Thermo-economic optimisation**
  - Investment estimation
  - Combined process integration and modelling
- **Multi-objective optimisation**
  - Efficiency - Investment
  - Pareto curve
- **Evolutionary algorithms**
  - Determine the value of P^*
- **Design evaluations**